We claim:

1. A crystal of an AR-LBD comprising:
   a) an AR-LBD and an AR-LBD ligand or
   b) an AR-LBD without an AR-LBD ligand;

wherein said crystal diffracts to at least 3 angstrom resolution and has a crystal stability within 5% of its unit cell dimensions.

2. The crystal of claim 1 wherein said AR-LBD has at least 200 amino acids.

3. The crystal of claim 1, wherein said AR-LBD is the AR amino acid sequence 672 to 917 of rat AR

4. The crystal of claim 1, wherein said AR-LBD is the AR amino acid sequence 672 to 917 of human AR.

5. The crystal of claim 1 wherein the crystal comprises an AR-LBD and an AR-LBD ligand and the AR-LBD ligand is an agonist or antagonist, a partial agonist or partial antagonist, or a SARMs of the AR-LBD.

6. The crystal of claim 5 wherein the agonist is dihydrotestosterone.

7. The crystal of claim 1 having all of the coordinates listed in Table A.

8. The crystal of claim 1 wherein said crystal comprises mammalian AR-LBD protein.

9. The crystal of claim 1 wherein said crystal comprises rat AR-LBD protein.

10. The crystal of claim 1 wherein said AR-LBD ligand has the following unit cell dimensions in angstroms: $a = 56.03 \pm 5\%$, $b = 66.27 \pm 5\%$, $c = 70.38 \pm 5\%$ and an orthorhombic space group P212121.

11. A molecule or molecular complex comprising all or any part of the ligand binding site defined by structure coordinates of AR-LBD amino acids V685, L700, L701, S702, S703, L704, N705, E706, L707, G708, E709, Q711, A735, I737, Q738, Y739, S740, W741, M742, G743, L744, M745, V746, F747, A748, M749, G750, R752, Y763, F764, A765, L768, F770, M780, M787, I869, L873, H874, F876, T877 and F878 according to Table A, or a mutant or homologue of said molecule or molecular complex.

12. The molecule or molecular complex of claim 11 wherein said mutant or homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said AR-LBD amino acids of not more than 1.5 Angstroms or 30% sequence identity with said AR-LBD amino acids.

13. A molecule or molecular complex comprising all or any part of the ligand binding site defined by structure coordinates of AR-LBD amino acids N705, Q711, R752, F764 and T877 according to Table A, or a mutant or homologue of said molecule or molecular complex.

14. The molecule or molecular complex of claim 13 wherein said mutant or homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said AR-LBD amino acids of not more than 1.5 Angstroms or 30% sequence identity with said AR-LBD amino acids.

15. A machine-readable data storage medium comprising a data storage material encoded with machine readable data, wherein the data is defined by the structure coordinates of an AR-LBD/AR-LBD ligand or ligand complex according to Table A or a homologue of said complex, wherein said homologue comprises backbone atoms that have a root mean square deviation from the backbone atoms of the complex of not more than 3.0Å

16. The machine-readable data storage medium according to claim 15, wherein said AR-LBD/AR-LBD ligand or ligand complex is homologue having a root mean square deviation from the backbone atoms of said amino acids of not more than 2.0 Å.

17. A machine-readable data storage medium comprising a data storage material encoded with a first set of machine readable data comprising a Fourier transform of at least a portion of the structural coordinates for an AR-LBD/AR-LBD ligand according to Table A; which, when combined with a second set of machine readable data comprising an X-ray diffraction pattern of a molecule or molecular complex of unknown structure, using a machine programmed with instructions for using said first set of data and said second set of data, can determine at least a portion of the structure coordinates corresponding to the second set of machine readable data, said first set of data and said second set of data.

18. A binding site in AR-LBD for an AR modulator in which a portion of said ligand is in van der Walls contact or hydrogen bonding contact with any portion or all of residues V685, L700, L701, S702, S703, L704, N705, E706, L707, G708, E709, Q711, A735, I737, Q738, Y739, S740, W741, M742, G743, L744, M745, V746, F747, A748, M749, G750, R752, Y763, F764, A765, L768, F770, M780, M787, I869, L873, H874, F876, T877, F878, L880, L881, V889, F891, P892, E893, M894, M895, A896, E897, I898, I899, S900, V901, Q902, V903, P904 or I906 of AR-LBD according to Table A.

19. The binding site according to claim 18 wherein the AR-LBD is a homologue or mutant with 25%-95% identity to residues V685, L700, L701, S702, S703, L704, N705, E706, L707, G708, E709, Q711, A735, I737, Q738, Y739, S740, W741, M742, G743, L744, M745, V746, F747, A748, M749, G750, R752, Y763, F764, A765, L768, F770, M780, M787, I869, L873, H874, F876, T877, F878, L880, L881, V889, F891, P892, E893, M894, M895, A896, E897, I898, I899, S900, V901, Q902, V903, P904 or I906 of AR-LBD according to Table A.

20. A method of obtaining structural information about a molecule or a molecular complex of unknown structure by using the structure coordinates set forth in Table A, comprising the steps of:

a. generating X-ray diffraction data from said crystallized molecule or molecular complex;

b. applying at least a portion of the structure coordinates set forth in Table A to said X-ray diffraction pattern to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex; and

c. using all or a portion of the structure coordinates set forth in Table A to generate homology models of AR-LBD or any other nuclear hormone receptor ligand binding domain.

21. A computational method of designing an androgen receptor synthetic ligand comprising:

a. using a three dimensional model of a crystallized protein comprising an AR-LBD/AR-LBD ligand complex to determine

at least one interacting amino acid of the AR-LBD that interacts with at least one first chemical moiety of the AR-LBD ligand; and

b. selecting at least one chemical modification of said first chemical moiety to produce a second chemical moiety with a structure that either decreases or increases an interaction between said interacting amino acid and said second chemical moiety compared to said interaction between said interacting amino acid and said first chemical moiety.

22. A method for identifying a compound that modulates androgen receptor activity, the method comprising any combination of steps of:

a. modeling test compounds that fit spatially into the AR-LBD as defined by structure coordinates according to Table A, or using a three-dimensional structural model of AR-LBD, mutant AR-LBD or AR-LBD homologue or portion thereof;

b. using said structure coordinates or ligand binding site as set forth in claim 18 to identify structural and chemical features;

c. employing identified structural or chemical features to design or select compounds as potential AR modulators;

d. employing the three-dimensional structural model or the ligand binding site to design or select compounds as potential AR modulators;

e. synthesizing the potential AR modulators;

f. screening the potential AR modulators in an assay characterized by binding of a test compound to the AR-LBD; and

g. modifying or replacing one or more amino acids from AR-LBD selected from the group consisting of V685, L700, L701, S702, S703, L704, N705, E706, L707, G708, E709, Q711, A735, I737, Q738, Y739, S740, W741, M742, G743, L744, M745, V746, F747, A748, M749, G750, R752, Y763, F764, A765, L768, F770, M780, M787, I869, L873, H874, F876, T877, F878, L880, L881, V889, F891, P892, E893, M894, M895, A896, E897, I898, I899, S900, V901, Q902, V903, P904 or I906 of AR-LBD according to Table A.

23. The method according to claim 22 wherein the potential AR modulator is from a library of compounds.

24. The method according to claim 22 wherein the potential AR modulator is selected from a database.

25. The method according to claim 22 wherein the potential AR modulator is designed *de novo*.

26. The method according to claim 22 wherein the potential AR modulator is designed from a known agonist, partial agonist, antagonist, partial antagonist or SARMs.

27. The method according to claim 22 wherein the potential AR modulator is an agonist or partial agonist and AR activity is measured by translocation or unwinding or helix 12.

28. The method according to claim 22 wherein the potential AR modulator is an antagonist or partial antagonist and AR activity is measured by translocation or unwinding or helix 12.

29. An AR modulator identified by the method of claim 22.

30. A method for treating prostate cancer comprising administering an effective amount of an AR modulator identified by the method of claim 22.

31. A method for treating an age related disease comprising administering an effective amount of an AR modulator identified by the method of claim 22.

32. The method of claim 31 wherein said age related disease is osteoporosis, muscle wasting or loss of libido.

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